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0.1 Molecular sets and representations of chemical reactions

A *uni-molecular chemical reaction* is represented by the natural transformations $\eta : h^A \longrightarrow h^B$, through the following commutative diagram:

$$\begin{array}{ccc} h^A(A) = Hom(A,A) & \xrightarrow{\eta_A} & h^B(A) = Hom(B,A) \\ \Big\downarrow{\scriptstyle h^A(t)} & & \Big\downarrow{\scriptstyle h^B(t)} \\ h^A(B) = Hom(A,B) & \xrightarrow[\eta_B]{} & h^B(B) = Hom(B,B) \end{array} \tag{0.1}$$

with the *states of molecular sets* $A_u = a_1, \ldots, a_n$ and $B_u = b_1, \ldots b_n$ being represented by certain endomorphisms in $Hom(A, A)$ and $Hom(B, B)$, respectively. In general, *molecular sets* M_S are defined as finite sets whose elements are *molecules* defined in terms of their molecular observables that are specified next. One need to define first the concept of a molecular class variable. A *molecular class variable*, or *m.c.v* is defined as a family of molecular sets $[M_S]_{i\in I}$, with I being an indexing set, or class, defining the *molecular range of variation* of the *m.c.v*. Most applications in Physics, Chemistry or Biochemistry require that I is a finite set, (that is, without any sub-classes). A *homomorphism of molecular sets* $M_t : M_S \to M_S$, with $t \in T$ being real time values, is defined as a time-dependent mapping or function $M_S(t)$ also called a M_t *molecular transformation*.

An *m.c.v. observable* of B, characterizing the products of chemical type "B" of a chemical reaction is defined as a morphism:

$$\gamma : Hom(B,B) \longrightarrow \Re,$$

where $\Re$ is the set or field of real numbers. This *mcv-observable* is subject to the following commutativity conditions:

$$\begin{array}{ccc} Hom(A,A) & \xrightarrow{f} & Hom(B,B) \\ \Big\downarrow{\scriptstyle e} & & \Big\downarrow{\scriptstyle \gamma} \\ Hom(A,A) & \xrightarrow[\delta]{} & R, \end{array} \tag{0.2}$$

with $c : A_u^* \longrightarrow B_u^*$, and A_u^*, B_u^* being, respectively, specially prepared *fields of states* of the molecular sets A_u, and B_u within a measurement uncertainty range, Δ, which is determined by Heisenberg's uncertainty relation, or the commutator of the observable operators involved, such as $[A^*, B^*]$, associated with the observable A of molecular set A_u, and respectively, with the obssevable B of molecular set B_u, in the case of a molecular set A_u interacting with molecular set B_u.

With these concepts and preliminary data one can now define the category of molecular sets and their transformations as follows.

0.2 Category of molecular sets and their transformations

Definition 0.1. The *category of molecular sets* is defined as the category C_M whose objects are molecular sets M_S and whose morphisms are molecular transformations M_t.

Remark 0.1. This is a mathematical representation of chemical reaction systems in terms of molecular sets that vary with time (or *msv*'s), and their transformations as a result of diffusion, collisions, and chemical reactions.

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